

Target Gas Density Calculator Concept, Usage & Limitations

NIF Users' Forum

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November 10, 2015



LLNL-PRES-710217

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

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Why Have a Gas Density Calculator?

- In 2012, it was realized that the non-ideality of subcritical THD gas mixtures exceeded the allowable uncertainty of the capsule density.
 - Why? Conversion from density to pressure was not accurate using the Ideal Gas Law alone.
 - Jim Fair authored the first calculator that calculated the density of the isotopic mixtures of hydrogen and helium.
 - Other gases & gas mixtures being shot are similarly non-ideal. E.g., Neopentane.
- Primary purpose
 - To calculate an accurate conversion of density (mg/cm^3) to pressure (torr) in target gas fill requests.
 - To quantify the non-ideal behavior of subcritical or high pressure gases and gas mixtures.
- Secondary purposes
 - To predict the equilibrium of THD mixtures (H_2 , D_2 , T_2 , HD, HT, DT) from cryogenic to room temperature.
 - To predict the atomic particle density (atoms/cm^3).

Model Approach To Non-Ideality Corrections

- Virial Coefficient Corrections to the Ideal Gas Law

- $z = \frac{P}{RT\rho_m} \approx 1 + B\rho_m + C\rho_m^2 + \dots$

- Mixing Rules (generally accepted for B, but not universally accepted for C)

- 2nd Virial Coefficient – for low pressure, low temp or moderate pressure, high temperature gases

- $B_{ij} = \frac{(B_i + B_j)}{2}$

- $B_{mix} = \sum_{i=1}^N y_i B_{ii} + \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N y_i y_j \delta_{ij}$

- $\delta_{ij} = 2B_{ij} - B_{ii} - B_{jj}$

- 3rd Virial Coefficient – for high pressure gases near critical temperature

- $C_{ijk} = \frac{(C_i + C_j + C_k)}{3}$

- $C_{mix} = \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N y_i y_j y_k C_{ijk}$

Caveats

- How good are the predictions? As good as the data.
 - E.g., Vapor pressure. Sources include:
 - Correlations from NIST
 - Compilation of literature data – polynomial fit
 - Antoine equation
 - THD Virial Coefficients
 - 2nd VC - High Confidence:
 - From PIMC models, which match historical data from Souers, Sherwood, Reed, Grilly and others, and is valid from 15K through RT.
 - 3rd VC - Unproven:
 - Is estimated using H₂ 3rd VC data and a corresponding states mapping (about T_r) from the 2nd VCs.
- Programming sanity checks is time consuming
 - Use your own judgment and knowledge of the materials being studied.
 - When in doubt, call me.

Using the Density Calculator (Demo)

- V2.5 & above:
 - On a PC: Open the document, accept that Macros need to be run.
 - Navigate to the “Calculator” tab.
 - Enter the desired mass density & shot temperature.
 - Adjust the composition.
 - Check the right hand fields.
 - Find the pressure alongside the desired composition

- V2.4 (Mac)
 - Open the document.
 - Navigate to the “Calculator” tab.
 - Enter the desired mass density & shot temperature
 - Adjust the composition.
 - For THD Mixtures ONLY:
 - N.B. Click the “THD Mixture Calculate” button. Wait for convergence.
 - If there is no convergence, navigate to the “THD EquilibriumCalculator” tab
 - Click “Reset” and “Solve” buttons.
 - Adjust “initial value factor” if necessary.
 - Re-click “Solve” to increase the number of solver iterations.
 - Check the right hand fields.
 - Find the pressure alongside the desired composition

- V2.6 beta
 - Working to resolve the issue of porting VB from PC to Mac version.

Using the Density Calculator (Demo)

- Case 1: Recent D₂-Filled HDC Symcap shot (N151025-001)
- Case 2: How do I request a specific density/mixture?
- Case 3: Post shot re-verification

Using the Density Calculator – Case 1

- Recent D₂-Filled HDC Symcap shot (N151025-001)
 - Original desired density:
 - 4 mg/cc at 32K
 - AppMan Request
 - 1486 Torr at 24K
 - Fielded Capsule
 - Liquid Deuterium
 - What red flags existed?

CryogenicTargetedDensity_PressureTest_v4.0_beta_mac.xlsx - Microsoft Excel

NOTE 1: You must press the "THD Mixture Calculate" button to calculate a THD_MIXTURE pressure
 NOTE 2: If you're working with THD mixtures and f_min is too large (RED), try going to THD_EquilibriumCalculator tab and adjust initial value factor +- 0.1 to find adequate minimum
 NOTE 3: The cell containing your desired pressure must be GREEN. A RED cell indicates some component pressure has exceeded it's vapor pressure at the specified density and temperature (i.e. it will

Input the desired density, temperature, and composition in PURPLE cells:

Desired mass density	4.000	(mg/cc=kg/m ³)
Shot temperature	32	(K)
Fraction D (for 3He+D2 mixtures)	0.3	(n.u)
THD_MIXTURE: Fraction T	0.50	(n.u)
THD_MIXTURE: Fraction H	0.00	(n.u)
THD_MIXTURE: Fraction D	0.50	(n.u)

Calculations involving T,H,D (including mixtures) valid for 15K < T < 300K
 Pure 3He and 4He calculations ok from 5K < T < 300K

THD Mixture Calculate f_min= 8.88E-16 <- If this cell stays RED, don't trust the calculated THD com

Atom densities

3He	7.987E+20	atom/cc
4He	6.018E+20	atom/cc
H	2.390E+21	atom/cc - Pure H2
D	1.196E+21	atom/cc - Pure D2
T	7.987E+20	atom/cc - Pure T2
3He+D	8.871E+20	atom/cc - Mixture
T	4.789E+20	atom/cc - Mixture
H	0.000E+00	atom/cc - Mixture
D	4.789E+20	atom/cc - Mixture
T+H+D	9.578E+20	atom/cc - Mixture

Pressure using Virial expansion:

Pure gases	3He	2668.2	(torr)	2nd virial
	4He	2003.5	(torr)	2nd virial
	H2	3387.7	(torr)	2nd virial
	D2	1814.1	(torr)	2nd virial
	T2	1244.1	(torr)	2nd virial
Mixtures	3He+D2	2467.5	(torr)	2nd virial, partial volume mixing
	THD_MIXTURE	1476.0	(torr)	2nd virial, partial volume mixing
		1969.7		

p/p_sat checks

	Psat	p_pure/Psat	p_mix/Psat
H2	8159.0	(torr)	0.42 0.00
D2	4840.4	(torr)	0.37 0.09
T2	3772.7	(torr)	0.33 0.11
DT	4273.4	(torr)	- 0.15
HD	6235.5	(torr)	- 0.00
HT	5548.0	(torr)	- 0.00

Ideal gas pressure:

3He	2646.7	(torr)	Ideal gas
4He	1994.3	(torr)	Ideal gas
H2	3960.3	(torr)	Ideal gas
D2	1981.7	(torr)	Ideal gas
T2	1323.3	(torr)	Ideal gas
3He+D2	2498.7	(torr)	Ideal gas, partial pressure mixing

NOTE 1: You must press the "THD Mixture Calculate" button to calculate a THD_MIXTURE pressure
 NOTE 2: If you're working with THD mixtures and f_min is too large (RED), try going to THD_EquilibriumCalculator tab and adjust initial value factor +- 0.1 to find adequate minimum
 NOTE 3: The cell containing your desired pressure must be GREEN. A RED cell indicates some component pressure has exceeded it's vapor pressure at the specified density and temperature (i.e. it will

Input the desired density, temperature, and composition in PURPLE cells:

Desired mass density	4.000	(mg/cc=kg/m ³)
Shot temperature	24	(K)
Fraction D (for 3He+D2 mixtures)	0.3	(n.u)
THD_MIXTURE: Fraction T	0.50	(n.u)
THD_MIXTURE: Fraction H	0.00	(n.u)
THD_MIXTURE: Fraction D	0.50	(n.u)

Calculations involving T,H,D (including mixtures) valid for 15K < T < 300K
 Pure 3He and 4He calculations ok from 5K < T < 300K

THD Mixture Calculate f_min= 1.85E-16 <- If this cell stays RED, don't trust the calculated THD com

Atom densities

3He	7.987E+20	atom/cc
4He	6.018E+20	atom/cc
H	2.390E+21	atom/cc - Pure H2
D	1.196E+21	atom/cc - Pure D2
T	7.987E+20	atom/cc - Pure T2
3He+D	8.871E+20	atom/cc - Mixture
T	4.789E+20	atom/cc - Mixture
H	0.000E+00	atom/cc - Mixture
D	4.789E+20	atom/cc - Mixture
T+H+D	9.578E+20	atom/cc - Mixture

Pressure using Virial expansion:

Pure gases	3He	1992.4	(torr)	2nd virial
	4He	1496.6	(torr)	2nd virial
	H2	2367.1	(torr)	2nd virial
	D2	1748.2	(torr)	2nd virial
	T2	897.9	(torr)	2nd virial
Mixtures	3He+D2	1823.9	(torr)	2nd virial, partial volume mixing
	THD_MIXTURE	1084.6	(torr)	2nd virial, partial volume mixing
		1459.4		

p/p_sat checks

	Psat	p_pure/Psat	p_mix/Psat
H2	1933.7	(torr)	1.10 0.00
D2	835.7	(torr)	1.54 0.37
T2	554.7	(torr)	1.62 0.56
DT	680.9	(torr)	- 0.63
HD	1267.0	(torr)	- 0.00
HT	1035.7	(torr)	- 0.00

Ideal gas pressure:

3He	1985.0	(torr)	Ideal gas
4He	1495.8	(torr)	Ideal gas
H2	2970.2	(torr)	Ideal gas
D2	1486.2	(torr)	Ideal gas
T2	992.5	(torr)	Ideal gas
3He+D2	1874.1	(torr)	Ideal gas, partial pressure mixing

Using the Density Calculator (Case 2)

- Case 2: How do I request a specific density/mixture?
 - 10 mg/cc of D₂ at 32K
 - Answer should be immediately available
 - 10 mg/cc of 0.4 at% D-³He at 32K
 - 10 mg/cc of 50:50 DT at 32K
 - Mac: must click solver button
 - 10 mg/cc of 2/24/74 HDT at 32K
 - Mac: must click solver button

Using the Density Calculator (Demo)

- Case 3: Post shot analysis
 - Requested: 10 mg/cc of 0.75/0.25 HT at 32K
 - Calculator indicates: 5022 Torr at 32K.
 - Cryo Reports on !DATA:
 - 5069 Torr
 - Mass Spec Analysis
 - 74% H
 - 25% T
 - 1% D
 - Calculator (trial & error)
 - 10.21 mg/cc at 32K
 - NOTE: 75/25 from calculator is 10.13 mg/cc

Current ELM Version is NIF-0135638-AF or v2.5

- Recently added/changed features
 - On the PC version, the THD Equilibrium Calculator is now “live,” no need to hit a reset & run-macro button
 - Seems to work for three-component THD mixtures.
 - Uses a pragmatic “forced-mass-balance” scheme to converge the equilibrium expressions.
 - Science fiction checks
 - Polynomial correlation of saturated vapor density of THD.
 - Color coding: an indication of when an estimate is violating something
 - **Green** is good
 - **Red** is bad
 - Any other color: **Use with Caution**
 - Data may be extrapolated or near some critical value (e.g., saturation temp, valid range of vapor pressure expression, etc.)
- If its broken, or if the calculator doesn't have a mixture or material that is of interest, contact me.